Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2024 – 08:03 AM EDT

PDB ID	:	3A3K
Title	:	Reversibly bound chloride in the atrial natriuretic peptide receptor hormone-binding domain
Authors	:	Ogawa, H.; Qiu, Y.; Ogata, C.M.; Misono, K.S.
Deposited on	:	2009-06-14
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

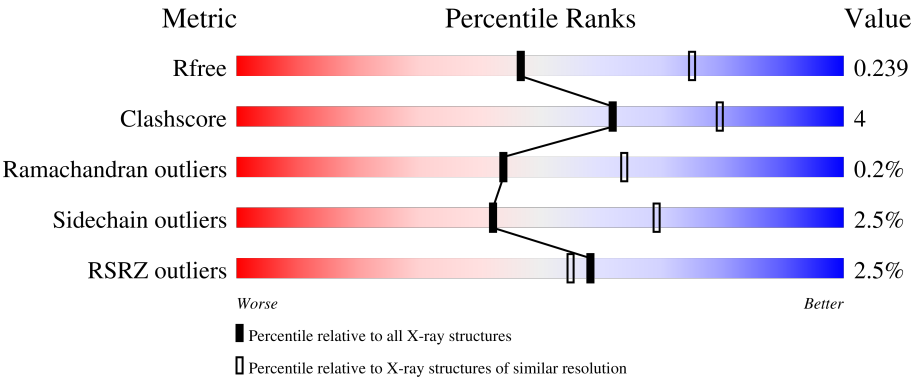
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	435	2% 88% 9%
1	B	435	3% 89% 9%
2	C	2	100%
2	D	2	100%
2	E	2	50% 50%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7189 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

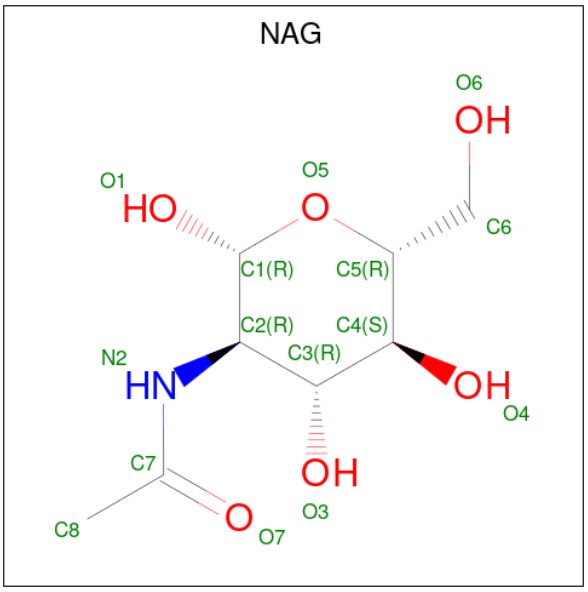
- Molecule 1 is a protein called Atrial natriuretic peptide receptor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	1	0
			3351	2150	583	607	11			
1	B	429	Total	C	N	O	S	0	1	0
			3389	2167	589	621	12			

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

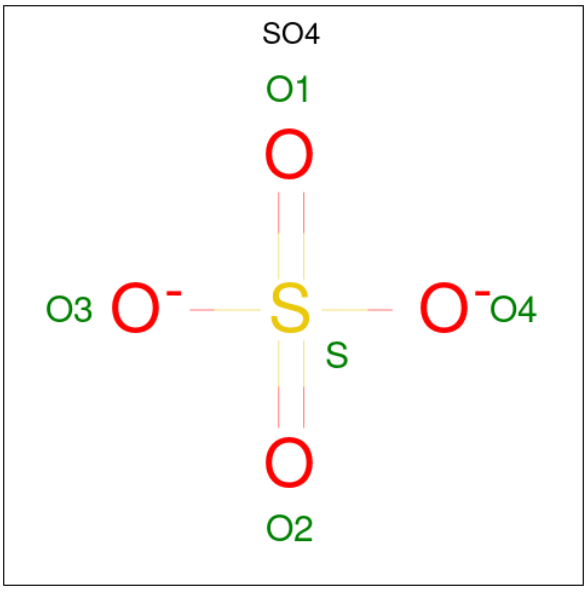
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

- Molecule 5 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Br 1 1	0	0
5	B	1	Total Br 1 1	0	0

- Molecule 6 is water.

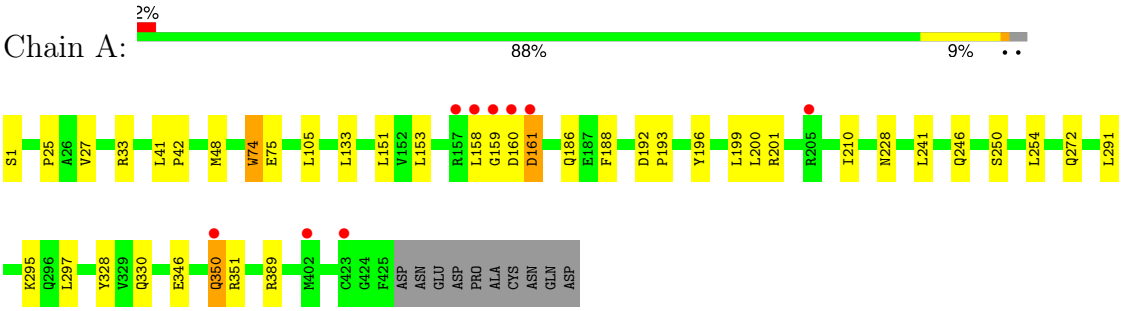
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	137	Total O 137 137	0	0
6	B	125	Total O 125 125	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

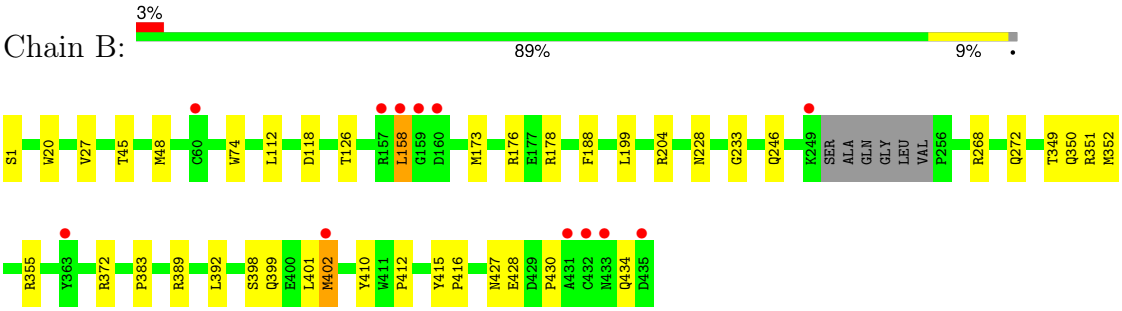
• Molecule 1: Atrial natriuretic peptide receptor A

Chain A:



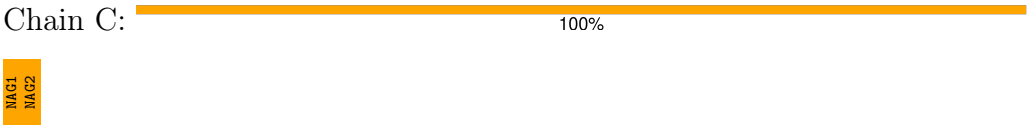
• Molecule 1: Atrial natriuretic peptide receptor A

Chain B:



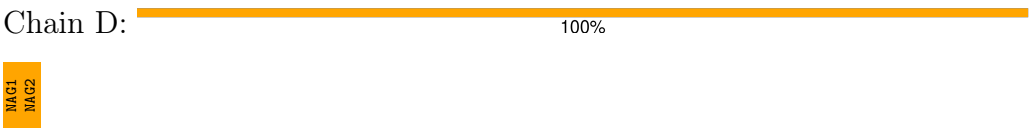
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	120.52Å 120.52Å 160.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.92 – 2.50 19.92 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.92-2.50) 92.3 (19.92-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.37 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.205 , 0.243 0.203 , 0.239	Depositor DCC
R_{free} test set	1936 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	26.2	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 28.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7189	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, SO4, BR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.86	10/3447 (0.3%)	0.78	12/4697 (0.3%)
1	B	0.76	10/3485 (0.3%)	0.81	8/4746 (0.2%)
All	All	0.81	20/6932 (0.3%)	0.80	20/9443 (0.2%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	74[A]	TRP	CG-CD1	-19.25	1.09	1.36
1	A	74[B]	TRP	CG-CD1	-19.25	1.09	1.36
1	B	74[A]	TRP	CG-CD1	-17.14	1.12	1.36
1	B	74[B]	TRP	CG-CD1	-17.14	1.12	1.36
1	A	74[A]	TRP	CD2-CE2	-16.75	1.21	1.41
1	A	74[B]	TRP	CD2-CE2	-16.75	1.21	1.41
1	B	74[A]	TRP	CD2-CE2	-12.20	1.26	1.41
1	B	74[B]	TRP	CD2-CE2	-12.20	1.26	1.41
1	A	74[A]	TRP	CD1-NE1	11.99	1.58	1.38
1	A	74[B]	TRP	CD1-NE1	11.99	1.58	1.38
1	B	74[A]	TRP	CD1-NE1	-10.86	1.19	1.38
1	B	74[B]	TRP	CD1-NE1	-10.86	1.19	1.38
1	B	74[A]	TRP	NE1-CE2	-6.96	1.28	1.37
1	B	74[B]	TRP	NE1-CE2	-6.96	1.28	1.37
1	A	74[A]	TRP	CG-CD2	6.64	1.54	1.43
1	A	74[B]	TRP	CG-CD2	6.64	1.54	1.43
1	A	74[A]	TRP	CD2-CE3	-5.62	1.31	1.40
1	A	74[B]	TRP	CD2-CE3	-5.62	1.31	1.40
1	B	74[A]	TRP	CG-CD2	5.06	1.52	1.43
1	B	74[B]	TRP	CG-CD2	5.06	1.52	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	74[A]	TRP	CD1-NE1-CE2	21.88	128.69	109.00
1	B	74[B]	TRP	CD1-NE1-CE2	21.88	128.69	109.00
1	A	74[A]	TRP	NE1-CE2-CZ2	-16.24	112.53	130.40
1	A	74[B]	TRP	NE1-CE2-CZ2	-16.24	112.53	130.40
1	A	74[A]	TRP	CD2-CE2-CZ2	14.09	139.20	122.30
1	A	74[B]	TRP	CD2-CE2-CZ2	14.09	139.20	122.30
1	B	74[A]	TRP	NE1-CE2-CD2	-13.72	93.58	107.30
1	B	74[B]	TRP	NE1-CE2-CD2	-13.72	93.58	107.30
1	A	74[A]	TRP	CD1-NE1-CE2	-8.67	101.19	109.00
1	A	74[B]	TRP	CD1-NE1-CE2	-8.67	101.19	109.00
1	B	74[A]	TRP	CG-CD1-NE1	-6.93	103.17	110.10
1	B	74[B]	TRP	CG-CD1-NE1	-6.93	103.17	110.10
1	B	74[A]	TRP	CD2-CE2-CZ2	6.90	130.58	122.30
1	B	74[B]	TRP	CD2-CE2-CZ2	6.90	130.58	122.30
1	A	74[A]	TRP	CE2-CD2-CG	6.75	112.70	107.30
1	A	74[B]	TRP	CE2-CD2-CG	6.75	112.70	107.30
1	A	74[A]	TRP	CH2-CZ2-CE2	-6.47	110.93	117.40
1	A	74[B]	TRP	CH2-CZ2-CE2	-6.47	110.93	117.40
1	A	74[A]	TRP	CE2-CD2-CE3	-5.08	112.61	118.70
1	A	74[B]	TRP	CE2-CD2-CE3	-5.08	112.61	118.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3351	0	3301	24	0
1	B	3389	0	3312	25	0
2	C	28	0	26	1	0
2	D	28	0	26	1	0
2	E	28	0	26	1	0
3	A	28	0	26	2	0
3	B	28	0	26	2	0
4	A	20	0	0	0	0
4	B	25	0	0	0	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
6	A	137	0	0	7	0
6	B	125	0	0	2	0
All	All	7189	0	6743	51	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (51) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:GLN:HG3	6:A:579:HOH:O	1.49	1.13
3:A:461:NAG:O4	3:A:462:NAG:C1	2.20	0.89
1:B:272:GLN:HG3	6:B:537:HOH:O	1.75	0.87
2:E:1:NAG:HO4	2:E:2:NAG:C1	1.97	0.77
1:B:233:GLY:HA3	1:B:412:PRO:HG2	1.65	0.77
1:B:178:ARG:HH22	1:B:399:GLN:HE22	1.31	0.75
1:A:161:ASP:HB2	6:A:553:HOH:O	1.87	0.75
1:A:330:GLN:HG2	6:A:490:HOH:O	1.87	0.74
1:B:415:TYR:HB2	1:B:416:PRO:HD2	1.72	0.71
3:B:461:NAG:O4	3:B:462:NAG:C1	2.44	0.65
1:B:27:VAL:HG11	1:B:48:MET:CE	2.29	0.62
1:A:160:ASP:HB2	6:A:553:HOH:O	2.01	0.61
1:A:74[B]:TRP:HD1	1:A:75:GLU:HG3	1.70	0.56
1:A:25:PRO:HB2	1:A:297:LEU:HD12	1.88	0.56
1:B:27:VAL:HG11	1:B:48:MET:HE1	1.86	0.56
1:A:228:ASN:ND2	1:B:204:ARG:HD3	2.22	0.55
1:A:196:TYR:CZ	6:A:436:HOH:O	2.60	0.54
1:B:427:ASN:HD22	1:B:434:GLN:NE2	2.05	0.54
1:A:228:ASN:HD21	1:B:204:ARG:HD3	1.72	0.53
1:A:27:VAL:HG11	1:A:48:MET:CE	2.38	0.53
1:A:200:LEU:HB3	1:B:228:ASN:OD1	2.10	0.52
1:B:392:LEU:HD13	1:B:401:LEU:HD22	1.92	0.51
1:A:291:LEU:O	1:A:295:LYS:HG3	2.10	0.51
1:B:427:ASN:HD22	1:B:434:GLN:HE21	1.57	0.51
1:B:349:THR:HA	1:B:352:MET:HE2	1.92	0.51
1:A:153:LEU:HD23	1:A:186:GLN:HB3	1.93	0.50
1:A:133:LEU:HD21	1:A:241:LEU:HD22	1.93	0.50
1:A:151:LEU:HD23	1:A:210:ILE:HD12	1.93	0.50
1:B:428:GLU:O	1:B:430:PRO:HD3	2.12	0.49
1:B:178:ARG:HH22	1:B:399:GLN:NE2	2.07	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:MET:HG3	6:B:565:HOH:O	2.12	0.49
1:A:105:LEU:HD11	1:A:328:TYR:HB2	1.94	0.49
1:B:178:ARG:NH2	1:B:399:GLN:HE22	2.07	0.48
1:A:346:GLU:HB2	6:A:485:HOH:O	2.12	0.48
2:D:1:NAG:C4	2:D:2:NAG:C1	2.91	0.48
1:A:188:PHE:CG	1:A:199:LEU:HD11	2.50	0.46
1:B:351:ARG:O	1:B:355:ARG:HD3	2.15	0.46
1:A:350:GLN:HG2	1:A:351:ARG:N	2.33	0.44
1:B:20:TRP:HH2	1:B:48:MET:HE1	1.82	0.44
1:A:196:TYR:CE1	6:A:436:HOH:O	2.57	0.43
2:C:1:NAG:C4	2:C:2:NAG:C1	2.95	0.43
1:A:105:LEU:HD11	1:A:328:TYR:CB	2.50	0.42
1:B:126:THR:O	1:B:372:ARG:HD2	2.20	0.42
1:A:41:LEU:N	1:A:42:PRO:HD3	2.35	0.42
1:B:398:SER:HB3	3:B:461:NAG:H61	2.01	0.42
1:B:188:PHE:CG	1:B:199:LEU:HD11	2.55	0.42
1:A:192:ASP:HA	1:A:193:PRO:HD3	1.89	0.41
3:A:461:NAG:C4	3:A:462:NAG:C1	2.98	0.41
1:A:201:ARG:NH2	1:B:268:ARG:HH22	2.18	0.41
1:B:112:LEU:HD22	1:B:173:MET:HG3	2.02	0.40
1:B:383:PRO:HG3	1:B:410:TYR:CD1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	424/435 (98%)	417 (98%)	6 (1%)	1 (0%)	44	64
1	B	426/435 (98%)	416 (98%)	9 (2%)	1 (0%)	44	64
All	All	850/870 (98%)	833 (98%)	15 (2%)	2 (0%)	44	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	158	LEU
1	A	159	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	353/361 (98%)	344 (98%)	9 (2%)	42	69
1	B	358/361 (99%)	349 (98%)	9 (2%)	42	69
All	All	711/722 (98%)	693 (98%)	18 (2%)	42	69

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	33	ARG
1	A	158	LEU
1	A	161	ASP
1	A	246	GLN
1	A	250	SER
1	A	254	LEU
1	A	350	GLN
1	A	389	ARG
1	B	1	SER
1	B	45	THR
1	B	118	ASP
1	B	158	LEU
1	B	176	ARG
1	B	246	GLN
1	B	350	GLN
1	B	389	ARG
1	B	402	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	228	ASN
1	A	246	GLN
1	A	272	GLN
1	B	185	HIS
1	B	296	GLN
1	B	399	GLN
1	B	434	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

6 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	C	1	2,1	14,14,15	0.65	0	17,19,21	1.23	1 (5%)
2	NAG	C	2	2	14,14,15	0.53	0	17,19,21	1.05	1 (5%)
2	NAG	D	1	2,1	14,14,15	0.64	0	17,19,21	1.16	2 (11%)
2	NAG	D	2	2	14,14,15	0.61	0	17,19,21	1.03	1 (5%)
2	NAG	E	1	2,1	14,14,15	0.60	0	17,19,21	1.28	3 (17%)
2	NAG	E	2	2	14,14,15	0.57	0	17,19,21	0.68	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	3/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1	NAG	C1-O5-C5	3.58	116.99	112.19
2	E	1	NAG	O5-C5-C6	2.99	113.48	107.66
2	C	2	NAG	C2-N2-C7	2.75	126.59	122.90
2	D	2	NAG	C1-O5-C5	-2.49	108.85	112.19
2	D	1	NAG	O4-C4-C3	-2.30	104.96	110.38
2	D	1	NAG	C3-C4-C5	2.27	114.35	110.23
2	E	1	NAG	C1-O5-C5	2.19	115.12	112.19
2	E	1	NAG	O5-C5-C4	-2.05	105.83	110.83

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C8-C7-N2-C2
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	D	2	NAG	C4-C5-C6-O6
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2

There are no ring outliers.

6 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	1	0
2	D	2	NAG	1	0
2	E	2	NAG	1	0

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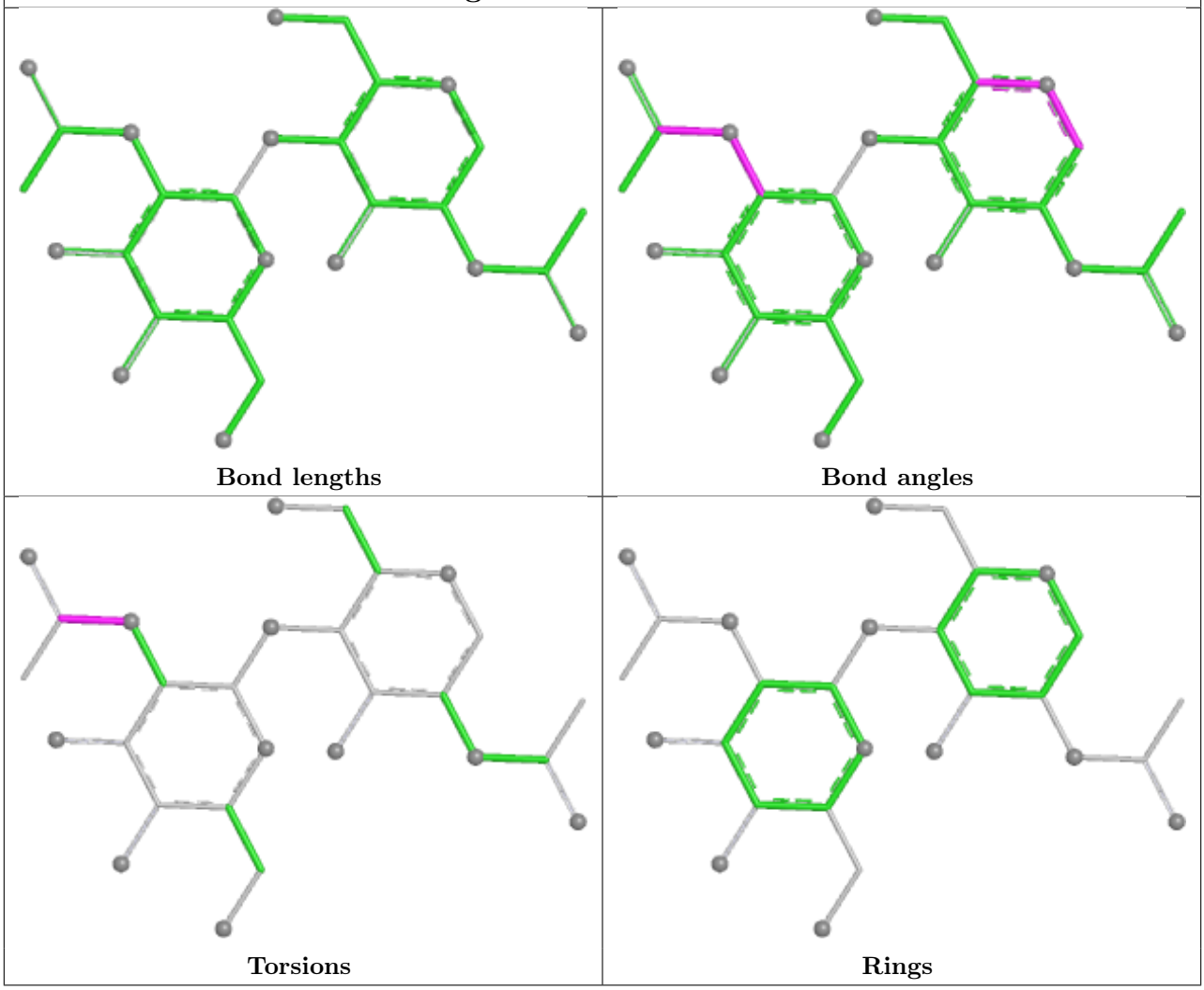
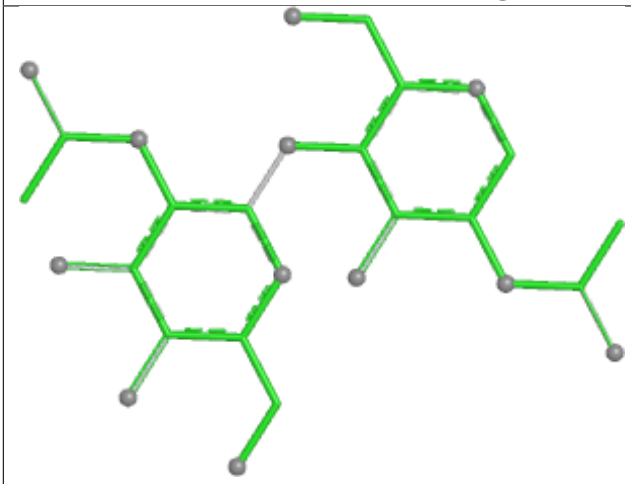
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	1	0
2	E	1	NAG	1	0
2	C	2	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

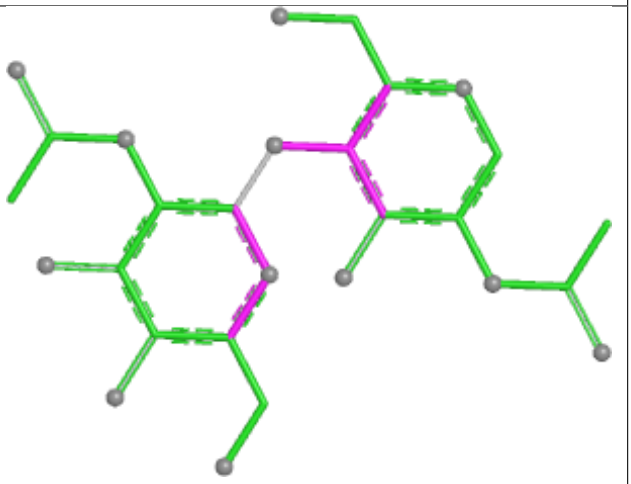
Oligosaccharide Chain C



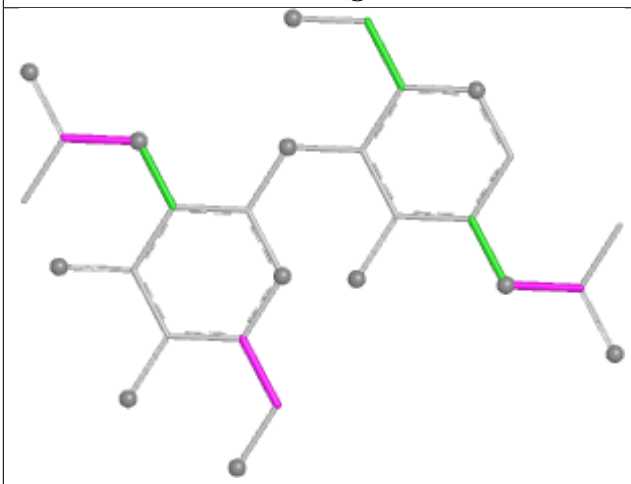
Oligosaccharide Chain D



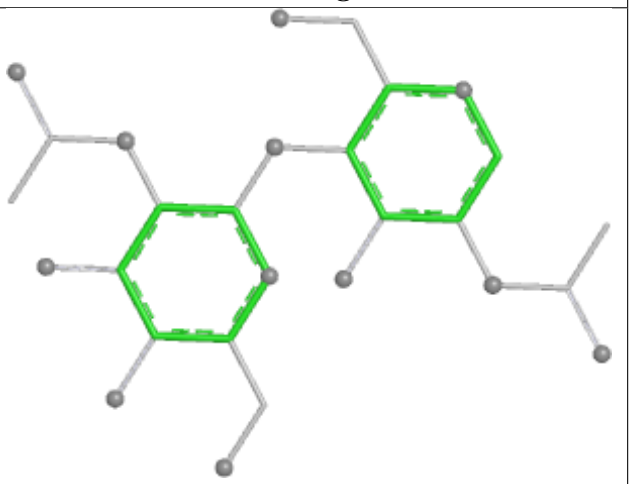
Bond lengths



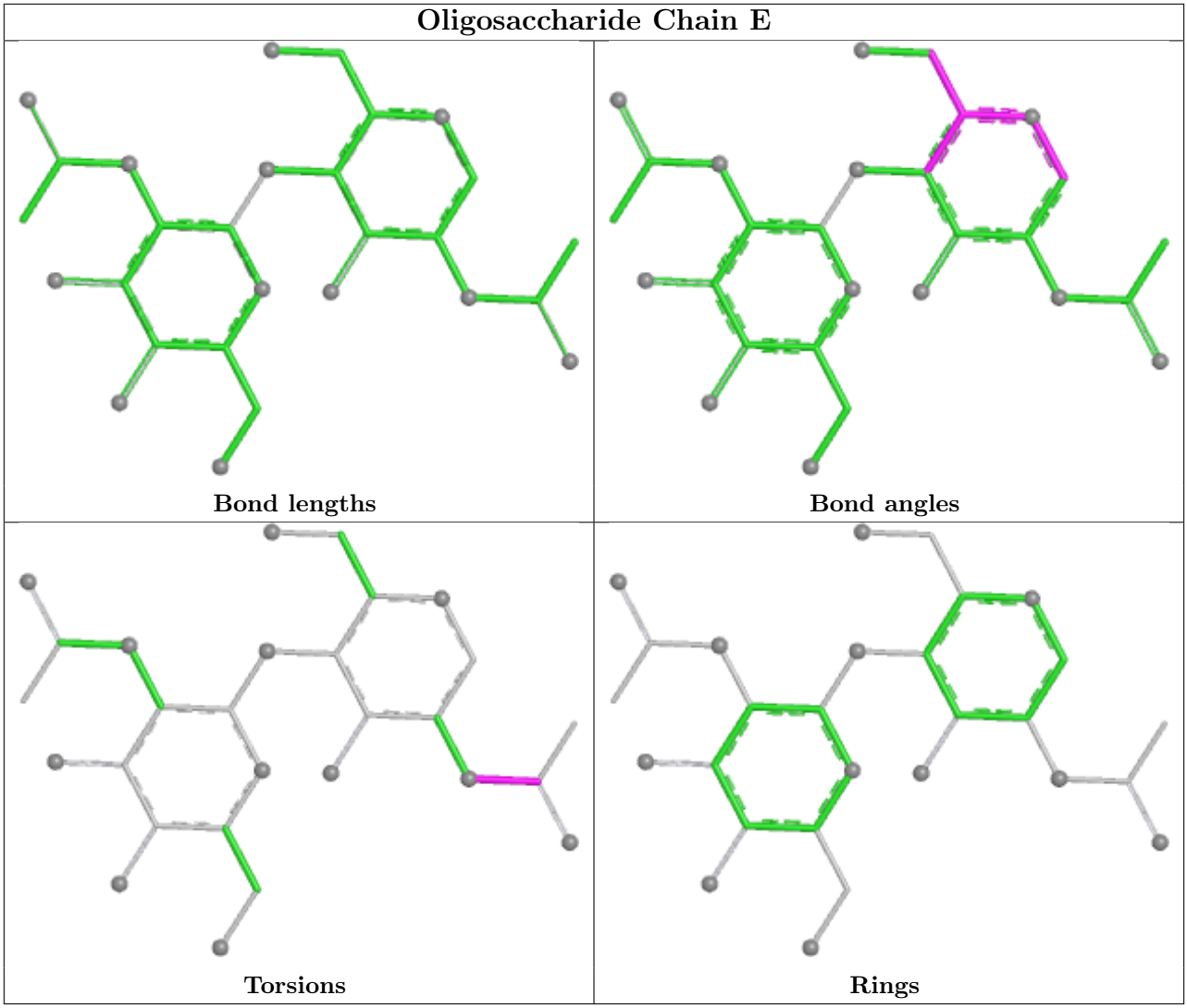
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	A	505	-	4,4,4	0.26	0	6,6,6	0.14	0
4	SO4	A	503	-	4,4,4	0.25	0	6,6,6	0.18	0
4	SO4	B	507	-	4,4,4	0.23	0	6,6,6	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SO4	A	501	-	4,4,4	0.22	0	6,6,6	0.35	0
3	NAG	B	461	1	14,14,15	0.66	0	17,19,21	1.65	3 (17%)
4	SO4	B	502	-	4,4,4	0.28	0	6,6,6	0.10	0
4	SO4	B	506	-	4,4,4	0.24	0	6,6,6	0.21	0
4	SO4	B	508	-	4,4,4	0.26	0	6,6,6	0.27	0
4	SO4	B	509	-	4,4,4	0.25	0	6,6,6	0.17	0
3	NAG	A	462	-	14,14,15	0.47	0	17,19,21	0.91	0
3	NAG	B	462	-	14,14,15	0.45	0	17,19,21	1.13	1 (5%)
3	NAG	A	461	1	14,14,15	0.68	0	17,19,21	0.99	1 (5%)
4	SO4	A	504	-	4,4,4	0.20	0	6,6,6	0.12	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	462	-	-	2/6/23/26	0/1/1/1
3	NAG	B	461	1	-	4/6/23/26	0/1/1/1
3	NAG	B	462	-	-	2/6/23/26	0/1/1/1
3	NAG	A	461	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	461	NAG	C1-O5-C5	3.99	117.53	112.19
3	B	461	NAG	C3-C4-C5	2.91	115.51	110.23
3	B	462	NAG	O5-C1-C2	-2.78	106.98	111.29
3	A	461	NAG	O4-C4-C3	-2.52	104.43	110.38
3	B	461	NAG	O5-C1-C2	-2.31	107.72	111.29

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	461	NAG	C8-C7-N2-C2
3	B	461	NAG	O7-C7-N2-C2
3	A	462	NAG	O5-C5-C6-O6
3	B	461	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	A	462	NAG	C4-C5-C6-O6
3	B	462	NAG	O5-C5-C6-O6
3	B	461	NAG	C4-C5-C6-O6
3	B	462	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	461	NAG	2	0
3	A	462	NAG	2	0
3	B	462	NAG	1	0
3	A	461	NAG	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	425/435 (97%)	-0.37	9 (2%)	63	60	10, 21, 36, 49	3 (0%)
1	B	429/435 (98%)	-0.34	12 (2%)	55	51	12, 23, 39, 61	3 (0%)
All	All	854/870 (98%)	-0.35	21 (2%)	58	55	10, 22, 37, 61	6 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	158	LEU	5.7
1	A	158	LEU	4.8
1	A	350	GLN	3.5
1	B	159	GLY	3.3
1	A	423	CYS	3.2
1	B	157	ARG	3.2
1	B	435	ASP	3.2
1	B	432	CYS	2.9
1	B	402	MET	2.8
1	A	161	ASP	2.8
1	B	433	ASN	2.8
1	A	159	GLY	2.6
1	A	160	ASP	2.5
1	B	160	ASP	2.5
1	A	402	MET	2.3
1	B	363	TYR	2.3
1	B	60	CYS	2.2
1	A	157	ARG	2.2
1	B	249	LYS	2.1
1	A	205	ARG	2.1
1	B	431	ALA	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

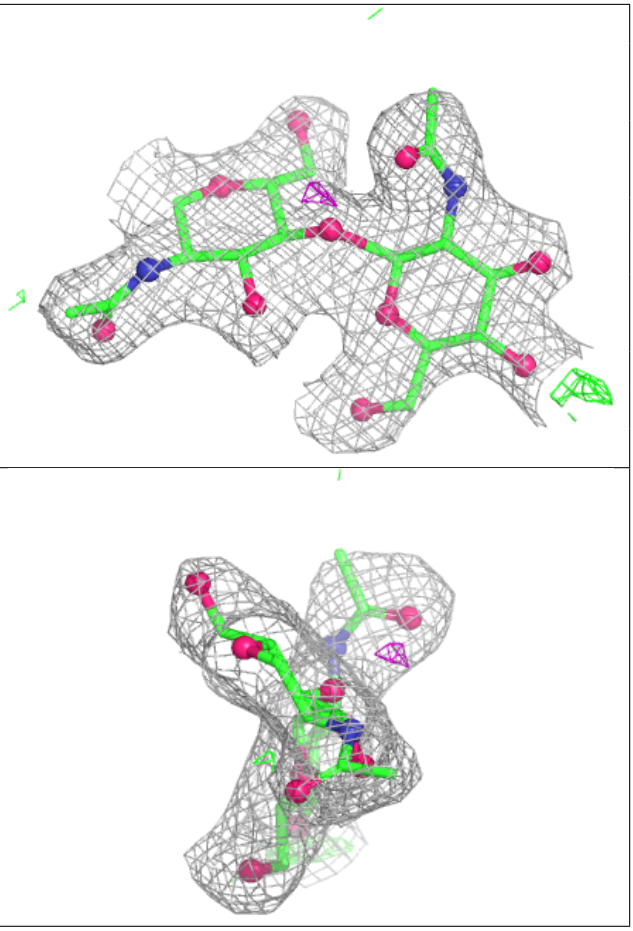
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	E	2	14/15	0.57	0.16	64,66,66,66	0
2	NAG	E	1	14/15	0.64	0.16	47,51,53,54	0
2	NAG	D	2	14/15	0.70	0.14	58,59,60,60	0
2	NAG	C	2	14/15	0.83	0.12	44,45,45,45	0
2	NAG	D	1	14/15	0.87	0.10	31,35,36,39	0
2	NAG	C	1	14/15	0.94	0.08	22,24,28,29	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

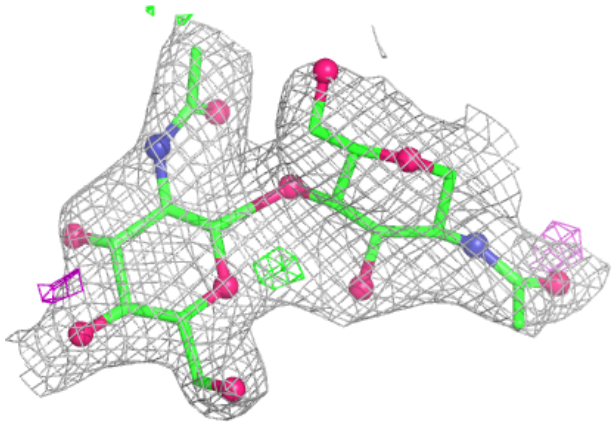
Electron density around Chain C:

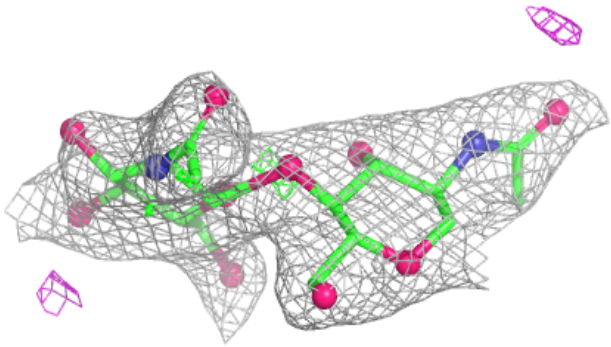
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

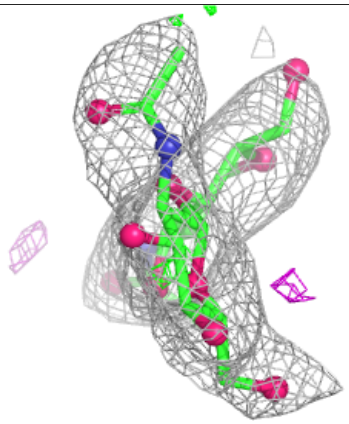


Electron density around Chain D:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

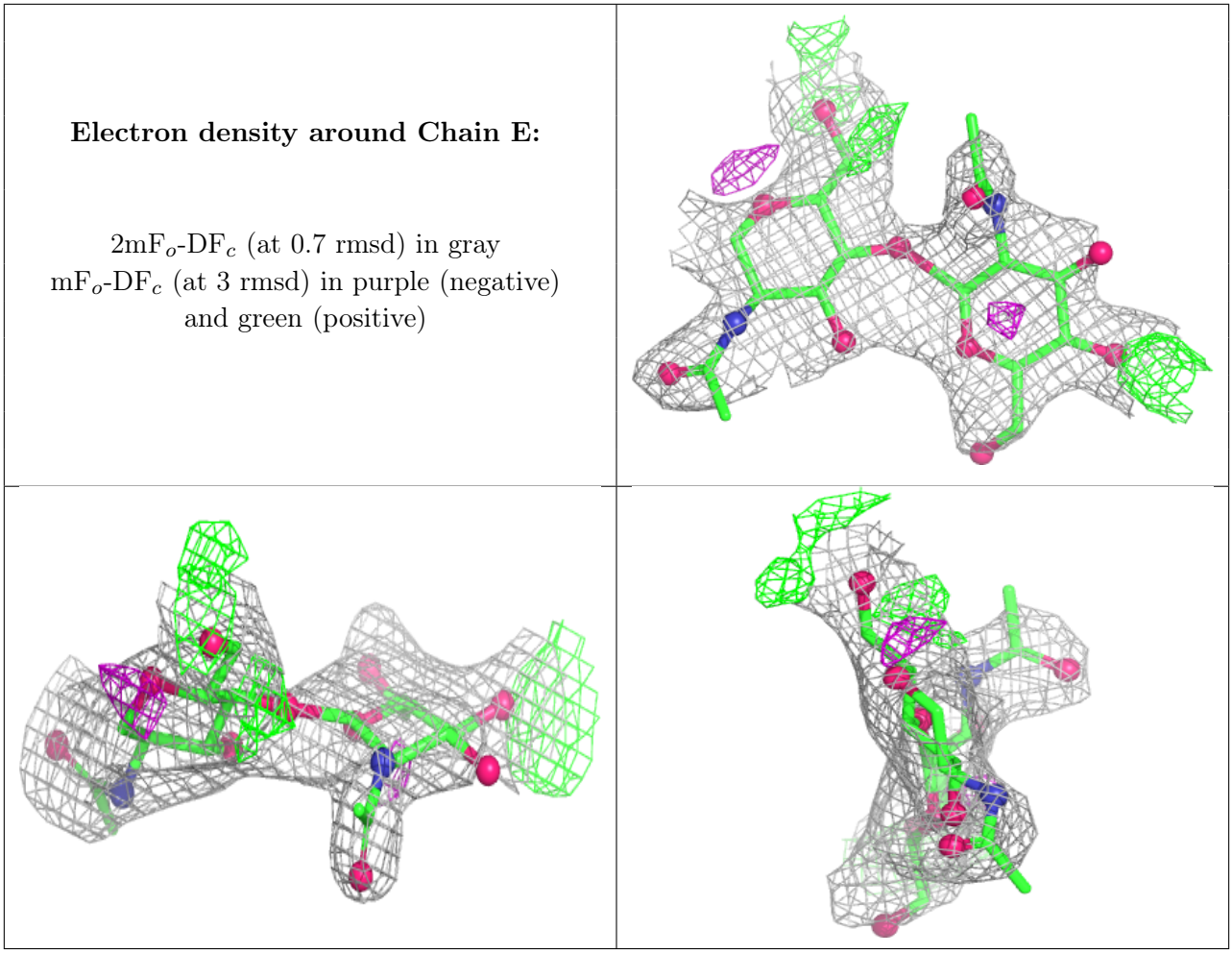






Electron density around Chain E:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	B	509	5/5	0.73	0.15	88,88,89,89	0
3	NAG	B	461	14/15	0.87	0.11	30,33,35,36	0
3	NAG	B	462	14/15	0.88	0.11	46,48,49,50	0
3	NAG	A	462	14/15	0.90	0.09	40,43,44,45	0
3	NAG	A	461	14/15	0.92	0.09	24,25,26,27	0
4	SO4	B	508	5/5	0.94	0.09	40,41,41,42	0
4	SO4	B	502	5/5	0.94	0.12	39,39,40,40	5
4	SO4	A	504	5/5	0.96	0.08	41,42,42,43	0
4	SO4	B	507	5/5	0.96	0.09	45,46,46,46	0
4	SO4	B	506	5/5	0.97	0.08	45,45,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	A	505	5/5	0.97	0.07	42,42,43,43	0
4	SO4	A	503	5/5	0.99	0.03	26,26,26,26	0
4	SO4	A	501	5/5	0.99	0.04	20,22,22,23	0
5	BR	A	600	1/1	1.00	0.07	21,21,21,21	0
5	BR	B	601	1/1	1.00	0.07	25,25,25,25	0

6.5 Other polymers (i)

There are no such residues in this entry.